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QUARTERLY PROGRESS REPORT:

INVESTIGATION OF KILOVOLT ION SPUTTERING

by

HAROLD P. SMITH, JR. AND F. C. HURLBUT

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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SPACE SCIENCES LABORATORY
UNIVERSITY OF CALIFORNIA, BERKELEY

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ABSTRACT

Final measurements have been made to assure that the cesium ion beam is focused and transported to the target without electron contamination or recombination. A more versatile lens system has been built to study the problem of mercury beam transmission, and an IBM 7094 computer program has been adapted to study the entrance conditions to the focusing lens assembly. Continued study of the cesium ion-copper sputtering has shown that reproducible results are obtained using the radioactive tracer technique. An additional computer program has been written for reduction of the angular distribution data. Construction and assembly of the mercury ion sputtering apparatus has continued. Various components of the time-of-flight apparatus have been tested. Finally, a computer program to simulate partially focused collision chains has been written and tested.

Author

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INVESTIGATION OF KILOVOLT ION SPUTTERING

by

Harold P. Smith, Jr. and F. C. Hurlbut

Space Sciences Laboratory, University of California, Berkeley

SUMMARY

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This report is submitted as a third quarterly progress report on our efforts to investigate sputtering of copper and molybdenum by kilovolt cesium and mercury ion beams, as well as to develop a time-of-flight technique for the measurement of the neutral sputtered particle velocity specturm. An additional theoretical study of partially focused crystallographic collision chains is included.

Final measurements have been made to assure that the cesium ion beam is focused and transported from the surface contact source to the target through a series of electrostatic lenses without significant electron contamination or recombination. The problem of focusing and transport of heavy ion beams in the KeV energy range has received additional study as a result of anticipated problems with the mercury ion beam which requires magnetic analysis. An adjustable lens system has been constructed and tested to study this problem. In addition, an IBM 7094 computer program has been adapted to our particular apparatus and is being used in conjunction with the experimental study. Actual construction of the mercury ion beam sputtering apparatus has proceeded on schedule.

Various components of a suitable time-of-flight apparatus have been investigated. The ultrahigh vacuum chamber has been able to attain

pressures in the low 10^{-10} Torr range, while a new ion source has been operated at greater than 100 microamperes. It was found that a small deflection chamber can successfully deflect the beam. However, fast chopping of the ion beam has not yet been tested although the pulsed power supplies have been built and tested. Some preliminary investigation of equipment for gating and counting has been made.

Finally, a computer program to simulate partially focused collision chains has been written. Preliminary results show that the program is working as expected but some problems remain. The primary difficulty is the slow rise in total energy in a system.

INTRODUCTION

Sputtering or ionic erosion of the accel electrode and focusing structure of the ion rocket engine can be the dominant mechanism limiting long term operation of the engine. Although the field of sputtering has been known since the phenomenon of gas discharge was first observed, no reliable theory to predict the yield, angular distribution, and velocity spectrum has been developed. Furthermore, it has only been within the past few years that experiments have been made under suitably defined conditions. In addition, there has been little work with either cesium or mercury beams so that it is difficult to predict the electrode erosion on the basis of previous data. For these reasons, the Lewis Research Center has sponsored detailed investigation of the sputtering of copper and molybdenum crystals under cesium and mercury ion beam bombardment where the target parameters such as temperature, angle of incidence, etc., are well known and varied over the range of interest.

The University of California (Berkeley) Space Sciences Laboratory began an investigation of this field early in 1964. Four vacuum systems have been constructed to study these effects using radioactive tracer techniques to measure the yield and angular distribution and mass spectrographic and time-of-flight analysis to determine the velocity spectrum of the various sputtered particles.

This report is submitted as a progress report on our continuing effort to develop suitable and versatile apparata for measurement of these phenomena. In addition, a theoretical investigation of one aspect of sputtering is considered.

It is a pleasure to acknowledge the valuable assistance of L. S. Stollar and J. Guthrie.

I. Ion Beam Transport*

Additional measurements of cesium ion beam transmission through a periodic electrostatic lens system have been made. The lens system was designed according to our application of P. K. Tien's[(1)] electron beam focusing analysis which was described in the last progress report. The apparatus is depicted in Figure 1.

Additional measurements were needed to insure that the cesium ion beam was suitably transferred to the target. A major concern was the contamination of the ion beam by secondary electrons created at negative potential lens surfaces by ion bombardment. Our previously reported calculations indicated that the contamination should be small. The calcu-

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* The work described in this section was performed by N. T. Olson, R. G. Musket, M. T. Stepp, and H. P. Smith, Jr.

(1) P.K. Tien, J. Appl. Phys., 25, 1281 (1954)

lations were checked experimentally by placing a biased transmission grid at the end of the lens stack. The usual positive current was measured when the grid was held at ground. Biasing the grid at a positive potential above that of the source prevented any ions from reaching the current measuring device. However, electrons in beam should be accelerated through the grid to the target. Carrying out this procedure indicated a small negative current which was less than 1/2% of the original positive current. Hence, it was concluded that some secondary electron contamination was taking place, but that it was well within acceptable limits of error.

Although our previous calculations indicated that electron-ion recombination was small, a measurement was made to check this. Again the biased grid was used to prohibit ion transmission to the target. However, any neutral components created by charge exchange or combination (and therefore at energies in the KeV region) would pass the grid and bombard the target. In this experiment, our usual radioactive copper target was used in order to detect any neutral component sputtering. As expected, there was no detectable copper sputtered from the target to the collector. Hence, it was concluded that any high energy neutral component in the beam was negligible.

A final measurement was made to detect whether there was significant beam spreading after the ion beam passed through the final lens and into the target-collector assembly. The distance from the lens to the target is of the order of 6 cm. Along this part of the ion path there are no lenses since there can be no obstruction between the target and the collector. During operation, the collector and target currents are summed in order to automatically compensate for secondary and photoelectron production in the target-collector assembly. Since this is the case, it is not possible to detect whether the spread of the ion beam is greater than the target diameter. For this particular measurement, the usual target was replaced by a series of small annular rings with an inner circle of diameter less than the usual target diameter. The current to each ring could be measured independently. The actual measurement showed that the current to the inner circle received over 99% of the ion current. The currents to the outer annular rings were at least two orders-of-magnitude less. It seems apparent from these results that the intense beam spreading at the ion source exit is associated with the acceleration and focusing at the ion source rather than with the space charge of the beam after it has been transmitted along the lens structure.

No further ion transmission problems or measurements for the cesium ion sputtering apparatus are anticipated. A report of this work has been prepared for journal publication.

The mercury ion sputtering apparatus which is being assembled presents a more complex problem of ion beam transmission than was encountered with the cesium apparatus. The mercury ion source is an electron bombardment type in which singly and multiply charged ions of any gaseous specie in the vacuum system can be created; whereas the cesium source was a surface ionization type in which only singly charged ions of cesium can be created. In order to insure that only singly charged mercury ions of known energy strike the target, it is necessary to incorporate a magnetic analyzer into the apparatus. Hence, the mercury beam must be focused and transmitted from the source to the magnet entrance, and from the magnet exit to the target. Obviously, electrostatic focusing cannot be used between the pole pieces of the magnet. Hence, the beam must be refocused at the magnet exit. In order to anticipate the problem of mercury ion beam transmission, a second, more versatile lens stack has been built to operate in our general test vacuum system. This stack allows independent voltage control and current measurement of each lens. Furthermore, the lens spacing can be chosen arbitrarily. Beam transmission up to eighteed inches can be tested in the present chamber.

Initial measurements using a cesium ion source similar to the one described previously, have been made, and the lens stack has been found to operate satisfactorily. The mercury source will be tested in the near future. However, an argon feed rather than mercury will be used for the initial runs . Assuming successful operation with argon, final test runs with mercury will be made.

A digital computer program, written under the direction of Professor T. Van Duzer of the University of California, Berkeley, Electrical Engineering Department, has been adapted to the conditions of our apparatus in order to study the ion beam optics at the entrance to the lens stack. As mentioned above, it seems that ion beam loss occurs primarily at the entrace to the lens stack. As mentioned above, it seems that ion beam loss occurs primarily at the entrace rather than in the periodic focusing portion of the stack. The program uses an iterative technique to determine the ion trajectories from the anode. Poisson's Equation is solved for an assumed perveance density and for a given electric potential on a closed boundary possessing radial symmetry. The ion trajectories are then computed from the electrostatic force field. A new perveance density is then computed and the process repeated until an acceptable agreement between iterations is obtained.

The results of this study simulating the cesium source with the first three lenses is presented in Figure 2. Two thousand mesh points were used and an accuracy of 10% between iterations was required. Inspection of Figure 2 shows that the part of the beam eminating from the center of the anode is intercepted. Since the emitting area is proportional to the radius in axial symmetry, this interception may be acceptable. However, further analytical work is anticipated to see if different spacing and voltages on the initial lenses will allow greater transmission. The analytic results will be checked using the experimental apparatus described above.

II. Cesium Ion Sputtering*

The technique and measurements described in the last progress report regarding the cesium-copper sputtering yield coefficient were continued. The technique seems to be sound and reproducible results were obtained. However, these preliminary measurements clearly demonstrate that the orientation of the ion beam with respect to particular crystallographic directions must be known to within at least one degreee. Although the von Laue back diffraction technique which we have used satisfactorily allows orientation of the crystal to within 1/2 degree, our previous irradiation procedure caused some misalignment (of the order of four degrees) between the crystal and holder. This problem has been resolved by building

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* The work described in this section was performed by N. T. Olson and H. P. Smith, Jr.

a special polyethlene irradiation capsule. No further problem in this regard is anticipated.

The angular distribution collection system has been completed and mounted in the target chamber. It consists of 100 small cubes of aluminum which present a 1 cm^2 area to the sputtered atoms from the target. (See Figure 3). The cubes are mounted directly opposite the target crystal and intercept approximately 70% of the 2 π sterradians in the hemisphere above the target. The rest of the solid angle is intercepted by aluminum foils. A foil also is placed in the plane of the target as shown in Figure 3. The need for the lower foil is discussed in a later paragraph.

The angular distribution is determined by applying our radioactive tracer technique to each cube. The laborious procedure of counting 100 radioactive samples is alleviated by use of an automatic sample changer with punch paper tape output which is automatically converted to IBM cards. Digital computer data reduction then provides the final information. The sample changer and its associated multichannel pulse height analyzer have been newly purchased. These instruments have been checked out and slightly modified. They are now ready for our particular use.

The computer program necessary for the data reduction has been written for use on the Berkeley Computer Center IBM 7094 computer. The program uses the method of Covell* to determine the relative number of counts in a particular gamma peak. (In the case of

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*D. F. Covell, U.S. Naval Radiological Defense Laboratory, Mare Island, California, Tech. Report 288.

copper, we examine the .511 MeV annihilation peak associated with the positron decay of Cu64). The more common technique of back stripping from the highest energy to the lowest, or the more sophisticated technique of selective stripping using linear programming and a library of known spectra is not needed for our particular work since only one radioactive specie is present and sufficient shielding is provided at the NaI crystal to assure that the background at the desired peak is adequately treated by Covell's method. In essence, this technique considers only those counts in a Guassian peak above an arbitrarily specified pulse width. This width is then held constant in comparing the activity of the various samples. The technique is ideally suited for the digital output of the pulse height analyzer since the pulse width can be specified by assigning a particular number of channels to the pulse. Covell has shown that the pulse need not be symmetric with respect to the channels chosen. Hence, data reduction can be quickly accomplished without the expense (and labor) of the more sophisticated methods.

In order for our angular distribution measurement technique to be correct it is necessary that the sticking probability of the copper atoms on the aluminum cubes be large. Preliminary measurements of the sticking probability have been made. A shadowed thermal beam of copper atoms was allowed to impinge on an aluminum block. The sharpness of the shadow object away from the beam indicated that the sticking probability was high. However, it is necessary to determine this effect under the conditions of our particular measurements. If the sticking probability for sputtered copper on to aluminum were equal to one, then inspection of the collection system shown in Figure 3 indicates that there would be no Cu64 activity detected on the lower foil (the foil in the plane on the target). Hence, counting of the lower foil provides a suitable check to determine whether significant bouncing occurs within the collector-target assembly and will therefore provide a suitable method for determining the accuracy of the angular distribution measurement. It should be noted that although we feel that the lower foil is an important part of the technique, we do not expect any difficulty associated with bouncing of the sputtered copper atoms.

Some difficulty has been experienced with our surface contact cesium ion source. Although the source has on occasion successfully produced over 100 microamperes of current at the first beam flag (see Figure 1), recent runs have been made in which the current is less than 0.1 microamperes. Further experimentation showed that the source cannot provide its rated current until approximately six hours after the source chamber has been under vacuum. After this delay, the source operates satisfactorily. It is assumed that the difficulty is associated with the residual gas in the delivery tube although the detailed effect is not clearly understood. However, a six hour delay between installation of the radioactive target and operation of the source does not seriously effect the technique.

Two further designs have now been incorporated in the apparatus. The lens stack has been adjusted according to our previously reported results and found to work very successfully. Secondly, the target holder is now equipped for liquid nitrogen cooling or operation with a hot air gun. This should allow operation between 100 and 700° K. In summary, it appears that the cesium sputtering apparatus is now ready for actual measurement of the yield and angular distributions of sputtered copper.

III. Mercury Ion Sputtering*

Construction and assembly of apparatus for mercury ion sputtering similar to that used for cesium ion sputtering is in process. This apparatus is, of necessity, more complex than the cesium apparatus as a result of the formation of multiple charged mercury ions and containant ions in the electron bombardment ion source. In order to insure that only single charged (or only doubly charged) mercury ions of known energy strike the target it is necessary to pass the ion beam through a bending magnet. The problem and associated investigation of ion beam focus and transport to and from the magnet chamber has been discussed in Section I. Further complexity results from the high gas load associated with the electron bombardment ion source as opposed to the surface contact cesium source. The main gas load in the target chamber is pumped by a six inch oil diffusion pump. A cryogenic baffle and gate valve are incorporated between the pump and the target chamber and additional cryogenically cooled surfaces are included in the target chamber itself to condense the neutral mercury component associated with mercury ion source operation. A high impedance to gas flow is created by the entrance and exit slits in the magnet chamber. The target chamber, where high vacuum is needed, is then separately pumped by a 100 ℓ/sec vac ion pump. All the parts necessary for the conversion of the pumping system from its previous use for the pulse counting measurements (see previous progress report) have been machined and assembled. The parts for the target and magnet chambers have been built and are in the process of being assembled. The design of the target chamber has been completed and construction of the necessary

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* The work reported in this section was performed by R.G. Musket and H.P. Smith, Jr.

parts is in process. The magnet and vac ion pump have been ordered.

The mercury ion source was recently delivered and will be tested in a separate vacuum system as described in Section I.

IV. Preliminary Measurements to Detect Sputtered Aluminum by Activation Analysis*

Recent successful testing of an ion rocket engine which used an aluminum accel electrode has indicated that aluminum may be able to withstand the sputtering associated with engine operation. For this reason, some preliminary measurements were made to determine whether the techniques which have been developed can be successfully applied to measurement of the yield and angular distribution of cesium (and mercury) sputtered aluminum.

Detection of sputtered aluminum particles by induced nuclear radiation calls for the development of a variation of our present technique. The only radioactive isotope of aluminum that can be formed by neutron irradiation of natural aluminum is Al 28 which emits both gamma and beta rays, but has a half-life of only 2.3 minutes. Hence, activation of the target before irradiation (the present technique) will have to be replaced by activation of a suitable collector containing the sputtered aluminum after ion bombardment. Recent preliminary measurements made at LPTR (Livermore Pool Type Reactor) demonstrated that neutron activation of natural aluminum was satisfactory for detection of 10 micrograms collected on standard polyethlene. No particular attempt was made to insure that the collector surface was clean. Hence, it seems likely that the sensitivity of the technique can be increased to detect one microgram

*The work reported in this section was performed by H. P. Smith, Jr.

quantities by using more suitable collectors such as graphite, milar, lead or titanium and improved handling techniques.

V. Velocity Spectrum Measurement Facility*

The ultra high vacuum system described in the previous progress report was chemically cleaned and then baked at 400°C for 24 hours. After cooling, the system pressure, read by a nude ionization gauge, reached 2×10^{-10} Torr. Inspection of the system showed that although most of the stainless steel parts were discolored, no serious deterioration seemed to have resulted from the high temperatures. The aluminum foil rotatable flanges seemed to perform perfectly under this severe treatment.

The quadrapole mass spectrometer was then incorporated in the vacuum system and the entire system was rebaked to 250° C. Inspection of the quadrapole ionizer showed discoloring of the various ceramic insulators but the resistive properties were intact. However, a number of spotwelds loosened during baking and had to be replaced. Furthermore, it was found that the ceramic vacuum wall feed-throughs were embrittled by the bakeout.** After replacement of the damaged feed-throughs, the mass spectrometer was again installed in the vacuum system but the bake-out process was temporarily deleted. Under these conditions the system operated at 2×10^{-8} Torr. Operation of the mass spectrometer ionizer initially raised the system pressure by an order of magnitude, but the system returned to the original pressure following approximately two hours of (non-continuous) operation. It was assumed that the initial pressure rise was associated with volatile species adsorbed on the ionizer

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*The work reported in this section was performed by D. W. DeMichele, H. P. Smith, Jr., and F. C. Hurlbut.

**This information was provided in the standard painful way that required installation of new feed-throughs.

surfaces which could be successfully boiled off merely by ionizer operation. The system will be operated at lower pressures during the next quarter to see whether the ionizer will constitute a gas load in the 10^{-9} Torr region. The initial results were encouraging in this regard. A short in the RF generator of the quadrapole electronics prevented immediate further work. Random pulse counting of argon introduced to the vacuum system through a controlled leak will follow successful operation of the mass spectrometer in the 10^{-9} Torr region.

Two cesium ion chopper assemblies have been built and are being tested. One, which was described in the previous report, uses a two-dimensional deflection system. Testing of this device was delayed as a result of not being able to obtain a suitable weld for the porous tungsten lens delivery tube. An additional cesium ion source has been obtained and has been tested using a split ring cylindrical chopper. A schematic of the chopper assembly and ion source is shown in Figure 4. Preliminary measurements using the test vacuum system indicate that the source with chopper attached can deliver over 100 μa to the target which is mounted on the same ultrahigh vacuum flange and can be positioned along the line of sight of the mass spectrometer. The deflection system is suitable for steady state deflection of the beam. However, the primary concern is whether the beam can be chopped so that 90% of the beam pulse can be contained within a one microsecond pulse width. The chopper pulse electronics have been built and tested. Fast repetitive ion beam chopping will be tested in the coming quarter.

In the past contract period increased attention has been given to the question of the data acquisition system for the velocity spectrum analysis of sputtered particles. The parent ion beam is to be moderated by deflection transverse to a slit system and then allowed to impringe on a target as a series of discrete pulses. The time lapse in the process of sputtering is of negligible magnitude in comparison with flight times of the sputtered particles (a point which, however, is subject o verification in the completed apparatus). Thus, knowing the velocity of the ion beam, one can establish the time of emergence of a pulse of the yield particles at the target. These then drift to the detector where they pass through the ionizer and mass filter and into the electron multiplier. A current pulse emerges, rising and falling in accordance with the spectrum of particle arrival times. When the signal to noise ratio permits, the arrival time spectrum may be observed directly in a scope presentation. However, where the noise is troublesome, and this possibility cannot be excluded, an integrating or information storage system must be employed.

Various elements of the system have been under study for some time. Under faculty research support an auxiliary vacuum system has been equipped for the study of ionizer and particle detector configurations and for the proofing of the external electronics. We are currently constructing a third ionizer assembly along lines proposed by Dr. Paul Scott, recently of MIT. Dr. Scott is viewed as a possible post-doctoral fellow in aeronautical sciences (ME) and may be of considerable assistance to the sputtering activity. At the present it would appear that a single information channel will be sufficient for the velocity spectrum analysis. Emphasis in signal handling design is currently placed on the gate timing apparatus and it now seems possible that a local supplier can produce a modification of a standard gate generator which would be well suited to our purpose. As an alternative, a versatile Techtronix scope (Model 547) has been shown to provide adequate sweep and delayed gates for repetitious recording of the sputtered particle arrival times. This model has a wide bandwidth and dual trace to allow simultaneous observation of the ion beam pulse as well as the electron multiplier ion pulse shape. The high speed counting scalers have already been purchased and tested. A low impedance pre-amplifier is being constructed which will be mounted directly at the electron multiplier output and should insure that the rise-time of the amplified electron multiplier pulses is considerably shorter than one microsecond.

It is hoped that the various components of the time-of-flight apparatus can be assembled during the next quarter in order that some preliminary data on sputtered particle velocity spectra can be obtained.

VI. Computer Simulation of Partially Focused Collision Chains*

When a crystal lattice is struck by high energy radiation, a rather large amount of kinetic energy can be transferred to a single atom. The initially struck atom then ploughs through the lattice striking other atoms and knocking them from their sites until its kinetic energy is dissipated. If the initial impact sends the primary atom in certain crystal directions, most of the kinetic energy can be transferred to the second atom. The primary atom replaces the second atom in its lattice site, and the second atom strikes a third atom. Collision chains can exist in crystal lattices which resemble collisions of billiard balls lined up in a row with a small separation between adjacent balls.

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*The work reported in this section was performed by Eric Jorgensen under the direction of H. P. Smith Jr. No charge to NAS 3-5743 is made; however, this effort is included in the progress report as a part of our investigation of sputtering.

Silsbee predicted focused collision chains in the < 110 > crystal direction. He pointed out that focusing occurs in an isolated, uniformly spaced straight line of hard spheres if the first sphere is projected toward the second at a small angle θ with the line of centers, and the separation of centers D is less than twice the diameter of the spheres. See Figure 1. Since atoms are not hard spheres, this focusing is likely to occur only at energies in which a modified hard sphere approximation is valid.

Gibson, Goland, Milgram, and Vineyard* confirmed the presence of collision chains in an elaborate study of radiation damage simulated on a computer. Gibson et al. considered a crystallite containing several hundred atoms which interacted with two body, central repulsive forces. Atoms on the surface were supplied with extra forces to simulate the reaction of an extended crystalline matrix. Events were started with all but one of the atoms at rest at their lattice sites. One atom was given an arbitrary kinetic energy and direction as though it had just been struck by a bombarding particle. They used a high speed computer to integrate the classical equations of motion:

$$\dot{v}_i(t) = m^{-1} F_i[x_1(t), x_2(t), \cdots x_N(t); v_i(t)]$$

$$\dot{x}_i(t) = v_i(t) \qquad\qquad i = 1, 2, \cdots, N$$

where N is three times the number of atoms in the set.

The results of the integration were printed out for various time intervals showing how the initially energetic atom transfers energy to neighboring atoms and how the kinetic energy ultimately is dissipated,

*Phys. Rev. 120, 1229 (1960).

and the set of atoms come to rest in a damaged configuration. Orbital plots of the motion of the atoms showed a strong tendency of energy to propagate along two lines of atoms: the close packed < 110 > line, as predicted by Silsbee, and the cubic < 110 > line. The model employed by Gibson et al. was considerably more complicated than Silsbee's isolated row of hard spheres. The row of atoms was imbedded in adjoining rows of atoms, and the moving atoms were continuously interacting with their neighbors under the influence of Born-Mayer forces.

It is noteworthy that the elaborate computer calculations produce collision sequences that have close qualitative resemblance to the chains given by Silsbee. The machine calculations showed that most of the energy is propagated along the chain; very little energy is lost to atoms in the neighboring chains. For a well-focused < 110 > chain with an energy of about 300 to 400 ev the energy lost by the atoms in the chain in forcing their way between neighbors was approximately 2/3 ev per step. The orbital plots show very little displacement of the neighboring chains as the energy is propagated down a < 110 > chain. Hence it is reasonable to postulate that the Gibson model can be simplified enormously in studying collision chains.

Since the elaborate machine computations of Gibson et al. show that a well-focused < 110 > chain does not produce any significant displacement of atoms in neighboring chains, one can greatly simplify computations on collision chains by considering all the neighboring atoms as fixed in place and calculating the motion of only the atoms in the chain. One can further simplify the model by considering only the motion down the chain. This one dimensional chain bounded by fixed neighboring atoms can be handled far more simply than Gibson's array.

The Gibson calculations frequently took hours of machine time, whereas the motion along the one dimensional chain can be computed in a few minutes. Moreover the mass of the individual atoms in the chain in the proposed model varied arbitrarily to simulate different isotopes or different atoms in the crystal.

The proposed model consists of a chain of atoms representing the < 110 > direction in a face-centered cubic crystal lattice. Atoms in the chain are allowed to move along the chain interacting with two body, central repulsive forces. Atoms alongside the chain are held fixed in place; however, they are allowed to interact and influence the motion of the atoms in the chain with the same two-body, central repulsive forces.

The forces used are based upon Born-Mayer potentials. The interaction energy of a pair of atoms separated by a distance r is given by

$$\phi = B e^{-\beta r} \tag{1}$$

This interaction describes the repulsion of atoms at distances of close approach. For convenience in specifying the constants in the Born-Mayer potential equation (1) is written in the form

$$\phi = A \exp\left[-\rho(r - r_0)/r_0\right]$$

where r_o is the near neighbor distance at zero pressure and absolute zero temperature. The constants A and in the Born-Mayer potential depend upon the interacting atoms. The distance r_o depends upon the equilibrium separation in the crystal.

Since the Born-Mayer potentials and hence the interaction forces between two atoms falls off exponentially with the distance, it is readily apparent that atoms at large distances from the chain need not be considered in determining the motion of the atoms along the chain. To illustrate we shall assume that the atom at (2, 2, 0) is struck and moves toward the lattice site (3, 3, 0). We shall calculate the potentials between the struck atom and the atoms which lie near the path from (2, 2, 0) to (3, 3, 0).

There are several combinations of constants in the Born-Mayer potentials. Gibson et al. list three sets which they used in their calculations. These are given in Table I.

TABLE I. CONSTANTS IN THE BORN-MAYER POTENTIALS

Potential	A (ev)	ρ
1	.0392	16.97
2	.0510	13.00
3	.1004	10.34

Since potential 3 gives the least rapid fall off with distance, we shall use it to determine approximately how far from the path of the struck atom that a neighboring atom must be before its influence is negligble. Table II lists the atoms nearest the path from (2, 2, 0) to (3, 3, 0) with their distance from the closest point on the path and the value of the exponential term in the Born-Mayer potential using $\rho = 10$.

TABLE II: ATOMS NEAR THE PATH FROM (2, 2, 0) TO (3, 3, 0)

Lattice Site of Neighboring Atom	Minimum Distance to Path, r	Value of Exponential $\exp\left[-10(r - r_o)/r_o\right]$
1, 1, 0	r_o	1
0, 2, 0	$\sqrt{2}\ r_o$	.0165
1, 3, 0	r_o	1
2, 4, 0	r_o	1
3, 5, 0	$\sqrt{2}\ r_o$	.0165
4, 4, 0	r_o	1
5, 3, 0	$\sqrt{2}\ r_o$	.0165
4, 2, 0	r_o	1
3, 1, 0	r_o	1
2, 0, 0	$\sqrt{2}\ r_o$	.0165
1, 2, 1	r_o	1
2, 3, 1	$(\sqrt{3}/2)\ r_o$	3.86
3, 4, 1	r_o	1
4, 3, 1	r_o	1
3, 2, 1	$(\sqrt{3}/2)\ r_o$	3.86
2, 1, 1	r_o	1
1, 2, -1	r_o	1
2, 3, -1	$(\sqrt{3}/2)\ r_o$	3.86
3, 4, -1	r_o	1
4, 3, -1	r_o	1
3, 2, -1	$(\sqrt{3}/2)\ r_o$	3.86
2, 1, -1	r_o	1
1, 4, 1	$\sqrt{2.75}\ r_o$	.0014
4, 1, 1	$\sqrt{2.75}\ r_o$	.0014
1, 4-1	$\sqrt{2.75}\ r_o$	.0014
4, 1-1	$\sqrt{2.75}\ r_o$	.0014

Atoms which are located at sites not listed in Table II are considerably farther away from the path and contribute even less to the motion of the atoms along the path.

The major component of the force on an atom in the chain comes from the atom behind and the atom in front along the chain. Since these atoms in the chain can move in closer than the distance r_o, their potential will increase rapidly and contribute far more to the force field on an atom in the chain than any neighbors. Hence the effect of neighboring atoms is comparatively quite small, and we shall consider only those which have a value of one or larger in the exponential term of the Born-Mayer potential.

The forces on any atom in the chain can be conveniently divided into the forces from the atoms in the chain and the forces from the sixteen nearest neighbors. Although the atoms which are two behind or two ahead of a given atom probably always will be too far away to contribute significantly to the force on the given atom, their influence will be included in the equations.

It is convenient to rotate the co-ordinate system 45^o in the z=0 plane, so that the x axis lines up with the $<110>$ close packed direction. The initial locations of all the atoms along the chain are given by the equation:

$$x_i = \left(\frac{i - r_o}{r_o}\right) \qquad i = 1, 2, \cdots, N$$

where N is the number of atoms in the chain. The neighboring atoms can also be specified in the new x - y coordiante system in terms of the standard unit r_o. We note that all the atoms in the z=0 plane can be specified in integral distances of r_o. The planes specified as $z=\pm 1$ in the old co-ordinate system are located a distance $r_o/\sqrt{2}$ above and below the z=0 plane. The x and y co-ordinates of the particles in these planes are specified by $(n+1/2)r_o$, where n can take on any integer value.

The force on the atoms is found by differentiating the Born-Mayer potential :

$$(F_i)_x = -\left(\frac{\partial\phi}{\partial r}\right)\frac{dr}{dx}$$

In our model we are considering the forces on the i-th atom in the chain contributed by the i-2, i-1, i+1, and i+2 atoms in the chain and the sixteen nearest neighboring atoms alongside the chain. These forces can be calculated individually and summed. The force in the new x direction on the i-th atom due to atom A is calculated below.

The distance between atom i and atom A is

$$r = \left[(x_i - x_A)^2 + (y_i - y_A)^2 + (z_i - z_A)^2\right]^{1/2}$$

This equation gives the force on i in the x direction resulting from the repulsive potential between i and A.

A computer program has been written which calculates the forces in the x, y, and z directions on each atom in the chain produced by the two atoms on each side of the given atom in the chain and by the sixteen nearest neighbors. The forces in each direction are summed separately to yield a net force in each direction for each atom in the chain. The equations of motion are numerically integrated using a standard Share-distributed subroutine, AIDE, (Automatic Integration of Differential Equation) which uses the Adams four-point formula.

The time steps used in the integration can be varied in the program and are determined by the maximum velocity and a preset fraction of the lattice spacing. This fraction has been varied from 1/4 to 1/1000 so that the time increments have been correspondingly the time for the fastest moving atom to traverse 1/4 to 1/1000 of the lattice spacing.

When the time steps are too large errors are introduced by allowing atoms to "gain" potential energy without losing kinetic energy. So far this problem has not been eliminated even by time steps corresponding to 1/1000 of the lattice spacing.

To date, chains of Cu63 set in the Gibson (Born-Mayer) Potential No. 2 have been simulated in the (100) plane of symmetry. The program seems to be performing correctly with exception to the slow rise in total energy of the system. It is hoped that this can be corrected in the near future. The accuracy of the assumptions can be checked against some of the particular solutions of Gibson, et al. Following this, a large variety of simulations can be made which should be interesting. Foremost among these is the simulation of focused chains in the alternating copper gold close-packed rows of fully ordered Cu_3Au.

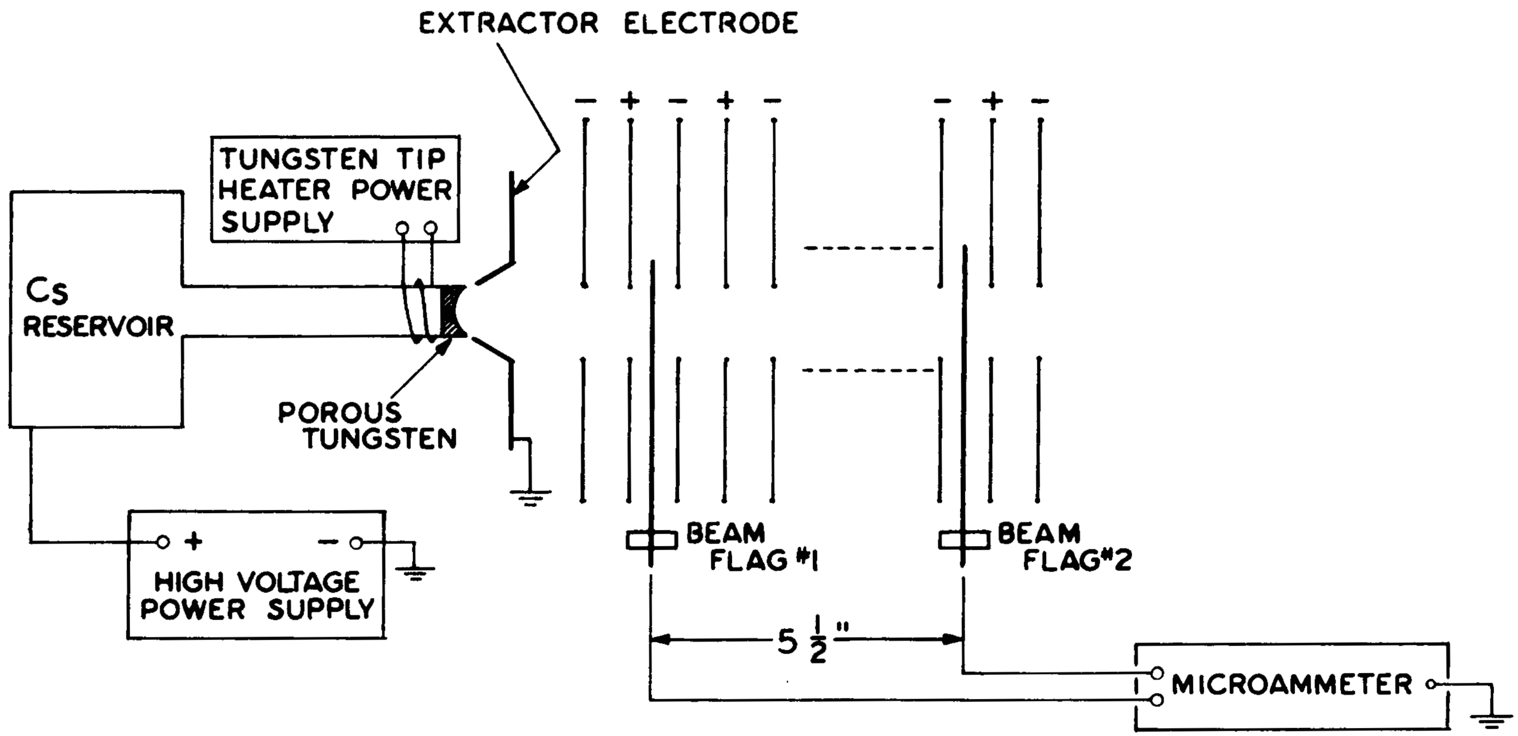

Figure 1: Schematic of cesium ion source and electrostatic focusing structure.

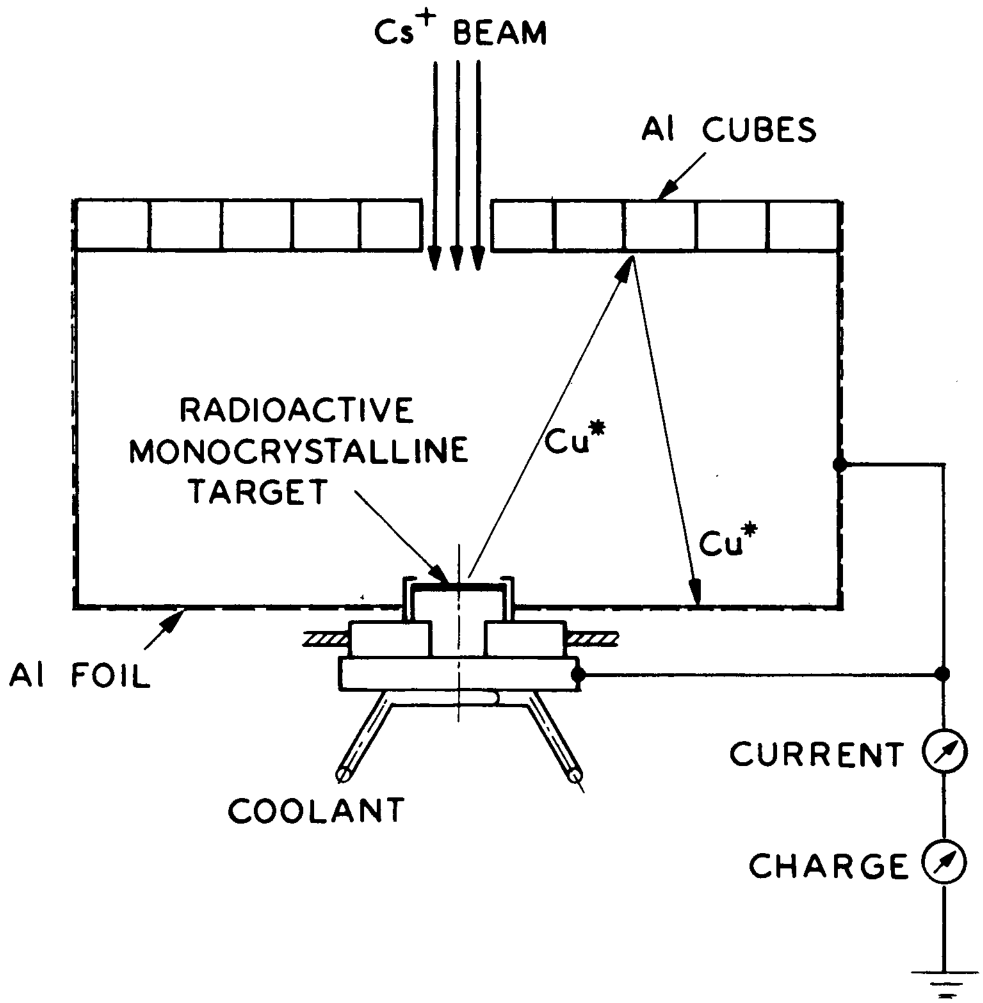

Figure 2: Schematic of target-collector assembly for measurement of the yield and angular distribution of sputtered copper. Detection of a sticking probability less than one is depicted.

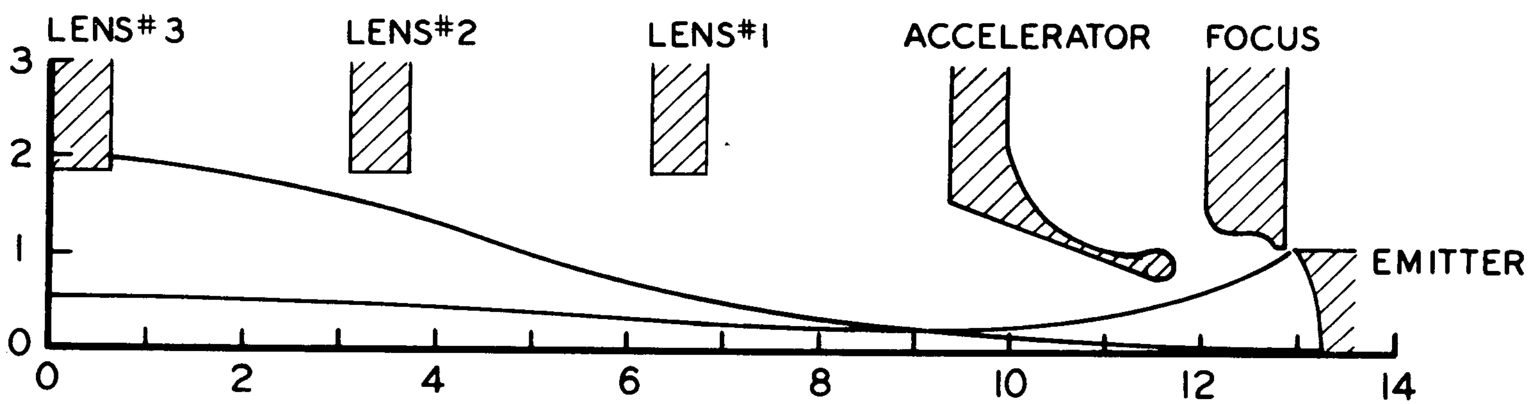

Figure 3: Computer simulation of ion trajectories for the cesium contact ion source and initial focusing structure.

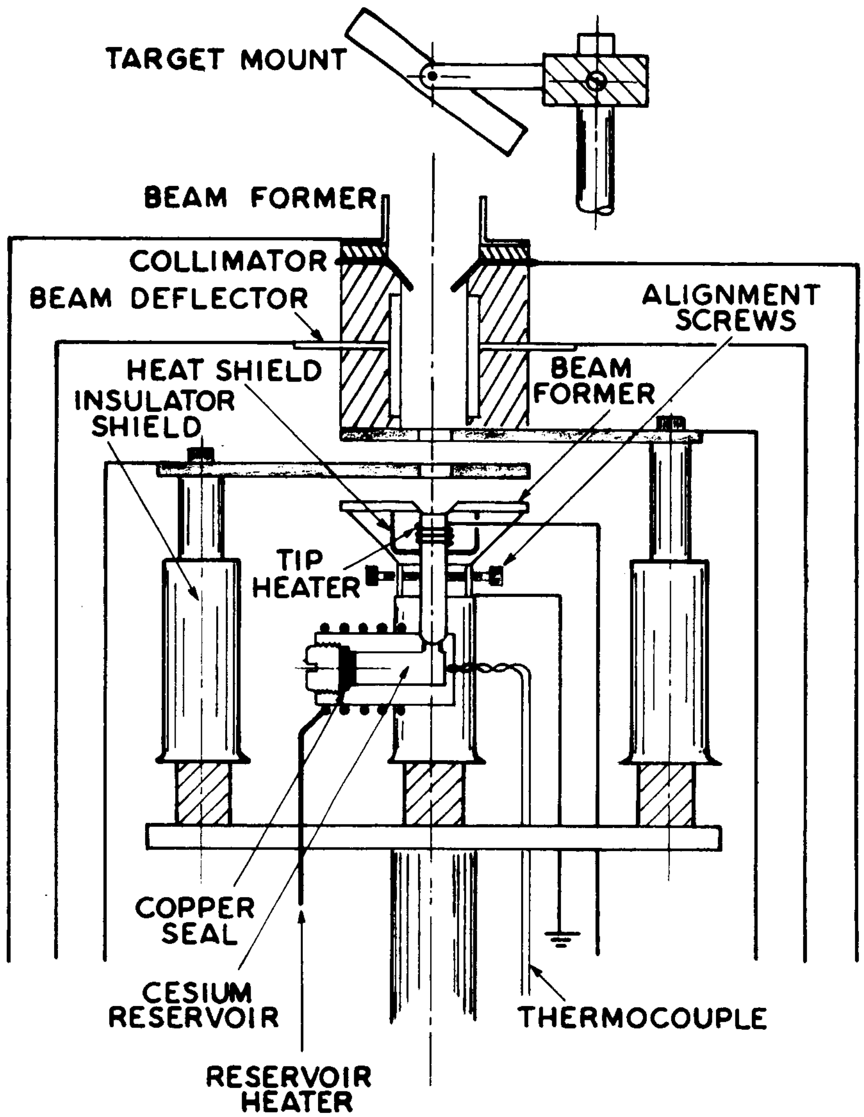

Figure 4: Schematic of ion source, beam deflector, and target mount for the time-of-flight apparatus.